

4H-Pyran-4-one, tetrahydro-3,5-bis(hydroxymethyl)-
67845-26-5 | DTXSID3028342

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.06

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 7.05e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethyl L-tartrate</div> <div>Measured: -0.290</div> <div>Predicted: -0.481</div>	<div>Image not found</div> <div>Pentaerythritol</div> <div>Measured: -1.69</div> <div>Predicted: -1.74</div>	<div>Image not found</div> <div>L-Ascorbic acid</div> <div>Measured: -1.85</div> <div>Predicted: -1.80</div>
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